COLLISION-INDUCED ROTATIONAL EXCITATIONS OF INTERSTELLAR MOLECULES DUE TO He AND H_2

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ABSTRACT.An Effective Straight-line Trajectory (EST) approach by introducing a parameter RX has been proposed[1] for computations of collision-induced rotational line widths (HWHM) and excitation rates in case of atom-molecule systems under the frame work of Smith, Giraud and Cooper[2] (1976) and molecule-molecule systems under the frame work of normalized semi-classical perturbative approach[3]. An optimised parameter RX, which is a measure of significance of the curved trajectories of the colliding molecules, can be determined from the temperature dependence of collision-induced line widths. The EST approach has been tested for HCl-Ar system and further applied to X-He and X-H_2 systems of interstellar interest, where X represents interstellar molecules CO,OCS and HCN. The results are given in Table I and II.

The conclusions drawn from the application of EST approach for computations of collision-induced rates are as follows:

a) The collision-induced rotational cross-sections using EST approach are within 5% to 16% with those of Smith et al[2] and within 0.6% to 14% with those of Robert and Bonamy[4], in case of HCl-Ar system.

b) The RX dependence of the rates in case of atom-molecule collisions is found to be more sensitive than molecule-molecule collisions.

c) The optimum trajectory corresponds to the optimum value of RX which may be determined using experimental informations. In this study the variation of line width with temperature has been used.

d) Information about the rates with perturber in excited rotational states ($J_2 \neq 0$) can also be determined which is very interesting since rotational population of interstellar molecules is found to be dependent on ortho and para states of interstellar H_2 .

e) The computer time required for EST method is only about 20% more than that required for straight-line trajectory approximation for computations of the rates. Hence due to its simple and non expensive nature the EST approach is expected to be more useful in the field.

f) The EST approach is not good for close collisions. The approximations in the potential surface does not allow to take into account the excitations with $\Delta J > 2$. The translational energy has been treated classically hence the approach can not be used at very low temperatures ($T < 50K$).

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Table I : Collision-induced rates ($cm^3\ S^{-1} \times 10^{10}$) for molecule-molecule systems using EST approach.

J_{2Jf}	J_i	CO-H_2			OCS-H_2			HCN-H_2		
		50°K	100°K	250°K	50°K	100°K	250°K	50°K	100°K	250°K
1	1-0	0.409	0.292	0.120	4.102	3.492	2.230	9.888	9.601	9.469
	2-1	0.499	0.359	0.146	4.276	3.730	2.452	10.311	10.030	9.918
2	1-0	0.300	0.210	0.087	3.743	3.094	1.860	9.015	8.942	8.898
	2-1	0.365	0.257	0.105	3.952	3.309	2.072	9.557	9.359	9.301
3.	1-0	0.280	0.196	0.082	3.647	3.016	1.776	8.822	8.828	8.791
	2-1	0.343	0.240	0.099	3.876	3.235	1.999	9.326	9.217	9.167
4	1-0	0.273	0.191	0.080	3.609	2.978	1.745	8.751	8.787	8.751
	2-1	0.335	0.234	0.096	3.846	3.201	1.971	9.251	9.165	9.118
5	1-0	0.269	0.188	0.079	3.590	2.958	1.730	8.731	8.767	8.733
	2-1	0.331	0.231	0.095	3.832	3.184	1.957	9.215	9.141	9.095

Table II : Line width parameters $\Delta\nu$ (MHz/torr) for atom-molecule systems using EST approach.

J_i — J_f	CO-He			OCS-He			HCN-He		
	50°K	100°K	300°K	50°K	100°K	300°K	50°K	100°K	300°K
1-2	7.007	4.297	1.576	12.910	5.730	1.500	11.541	7.099	3.567
2-3	6.963	4.209	1.571	12.335	5.619	1.522	8.718	5.523	2.350

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